Interface roughness and planar doping in superlattices: weak localization effects

George Kastrinakis
Institute for Electronic Structure and Laser (IESL), Foundation for Research and Technology - Hellas (FORTH), Iraklio, Crete 71110, Greece[*]

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We examine the effects of interface roughness and/or planar impurity doping in a superlattice, in the frame of a weak disorder description. We find that these two types of disorder are equivalent, and that they can be viewed as effective "bulk" disorder, with anisotropic diffusion coefficients. Our results offer quantitative insight to transport properties of multilayers and devices, which contain inadvertently structural disorder at the interfaces.

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We consider a superlattice composed of two materials A and B, each forming layers of thickness a and b along the $\hat{z}$ axis. The period of the superlattice along the same direction is $d = a + b$. In a perfect superlattice the electrons feel a periodic potential along the z direction, while they move freely in the xy plane. Hence we write the eigenfunctions as products of plane waves in the xy planes times Bloch functions along $\hat{z}$:

$$H_o \Psi_{knq} = \epsilon_{knq} \Psi_{knq} \quad , \Psi_{knq}(\mathbf{r}) = e^{i\mathbf{k}\rho} \Phi_{nq}(z) \quad , \Phi_{nq}(z) = e^{iqz} u_{nq}(z) \tag{1}$$

Here $\mathbf{k}, \rho \perp \hat{z}, \mathbf{q} \parallel \hat{z}, -\frac{\pi}{d} \leq q \leq \frac{\pi}{d}, \epsilon_{knq} = \epsilon_k + \epsilon_{nq}, \epsilon_k = \frac{k^2}{2m}, \epsilon_{nq}$ being the dispersion relation of the n-th band, with a bandwidth w_n, n running from 1 to n_b. Also, $u_{nq}(z) = u_{nq}(z + ld), l \in N$. Henceforth we will use k, K and q, Q to denote momenta perpendicular and parallel to $\hat{z}$, respectively.

We consider the effects of scattering either from the roughness of the interfaces between the two materials forming the superlattice or from 'impurities' (dopants) situated in planes parallel to the interfaces, i.e. vertical to the growth direction z. In this last case, and for charged dopants, we assume that their concentration is low enough so that the electronic distribution remains unaltered around the planes. Nevertheless, with a trivial modification in our expressions for the self energy and the Cooperon[1] our results are also valid for arbitrary kind of low doping.

We only consider spinless disorder, and we model the scattering potential with

$$V_s(\mathbf{r}) = \sum_i V_i(\rho) \delta(z - z_i) \quad , \tag{2}$$

where i runs over the interfaces/planes in consideration. $V_i(\rho)$ describes the roughness/doping profile respectively of the i-th interface/plane. Henceforth we will use the term 'plane' to denote both. This type of potential has been used before for the study of surface[2,3] and interface[4] effects.

Consequently, the Hamiltonian of the superlattice is given by

$$H = H_o + V_s \quad . \tag{3}$$

Our perturbative approach consists in treating V_s to lowest order. To this end, we calculate its matrix elements between the states $|knq\rangle$ corresponding to (1) above. For the sake of simplicity we assume that there is only one scattering plane per period (situated in the same relative position c). In fact, this is a very realistic possibility, as it often happens that only one of the two interfaces is rough, e.g. as in GaAs/AlGaAs superlattices. We will discuss the case of two planes per period after deriving the expression for the Cooperon. We obtain

$$V_{knq,k'n'q'} = \sum_i V_i(\mathbf{k'} - \mathbf{k}) \; \Phi^*_{nq}(c) \Phi_{n'q'}(c) \quad , \tag{4}$$

where $V(\mathbf{k})$ is the Fourier transform of $V(\rho)$. There is no correlation between different planes, i.e.

$$< V_i(k) V_j(k) >= \delta_{ij} < V^2(k) > \quad . \tag{5}$$

The bare Green's function here is

$$G^{R,A}_{on}(k, q, \epsilon) = \frac{1}{\epsilon - \epsilon_k - \epsilon_{nq} \pm i\delta}, \quad \delta \to 0^+ \quad . \tag{6}$$

The Dyson equation is

$$G_{nm} = G_{on}\delta_{nm} + \sum_l G_{on}\Sigma_{nl}G_{lm} \quad , \tag{7}$$

where the labels (k, q, ϵ) are implied.

To lowest order, the self-energy $\Sigma_{nl}(k, q, \epsilon)$ is given by

$$\Sigma_{nl}(k, q, \epsilon) = \Phi^*_{nq}\Phi_{lq} \sum_{m,k',q'} |V(k-k')|^2 G_{om}(k', q', \epsilon)|\Phi_{mq'}|^2 \quad , \tag{8}$$

where we have dropped the argument c from Φ. In the foregoing we take $V^2 =< |V(k)|^2 >$.

Setting $\sigma_{nq} = Im\,\Sigma_{nn}(q)$, we assume that $\epsilon_F - w_n \gg \sigma_{nq}$, which is the condition $\epsilon_F\tau \gg 1$ in weak localization. We further assume that the Fermi energy is bigger than the bandwidths w_n, in the sense that $\epsilon_F - w_n = O(\epsilon_F)$.

Henceforth we take

$$\varepsilon_{nq} = \epsilon_{nq} + \Re\,\Sigma_{nn}(q) \quad . \tag{9}$$

First, we give the Drude part of the static conductivity. For the in-plane conductivity we have ($\hbar = 1$)

$$\sigma_{xx} = \frac{2e^2}{\pi}\sum_n \int \frac{dq\ (\epsilon_F - \varepsilon_{nq})}{\sigma_{nq}} \quad , \tag{10}$$

while for the conductivity along $\hat{z}$ we have

$$\sigma_{zz} = \frac{2\ m\ e^2}{\pi}\sum_n \int \frac{dq\ \epsilon'^2_{nq}}{\sigma_{nq}} \quad , \tag{11}$$

the prime denoting differentiation with respect to q. Note that this expression, as well as the one for $\delta\sigma_{zz}$ below, behave correctly as the system becomes 2-dimensional. This is the case in which one material is insulating and forms a thick enough layer. As the insulating layer becomes thicker the dispersion of the mini-bands increasingly flattens-out, and hence $\epsilon'_{nq} \to 0$, yielding a decreasing conductivity along $\hat{z}$.

Next, in order to obtain the terms arising from the impurity-induced electron-hole correlation, we have to calculate the Cooperon first. The low-field dependence of the conductivity is entirely due to these terms. In analogy with ref.[2] we find for low temperature T

$$C_{q,nmrs}(K, Q, \omega) = V^2\Phi^*_{nq}\Phi_{mq}\Phi^*_{r,Q-q}\Phi_{s,Q-q}\ C(K, Q, \omega) \tag{12}$$

with

$$C(K, Q, \omega) = \frac{1}{1 - V^2\sum_{k,q,nmrs} G^R_{nm}(k, q, \epsilon_F + \omega)G^A_{rs}(K-k, Q-q, \epsilon_F)\Phi_{nq}\Phi^*_{mq}\Phi_{r,Q-q}\Phi^*_{s,Q-q}} \quad . \tag{13}$$

Assuming that there is reflection symmetry along the z direction, we evaluate $C(K, Q, \omega)$ for small K, Q, ω to obtain

$$C(K, Q, \omega) = \frac{1}{\mathcal{D}K^2 + \mathcal{D}_z Q^2 - i\omega L} \quad , \tag{14}$$

with

$$\mathcal{D} = \frac{t^2}{4m\pi\ S^3}\int dq \sum_n \frac{\epsilon_F - \varepsilon_{nq}}{|\Phi_{nq}|^2} \quad , \tag{15}$$

$$\mathcal{D}_z = \frac{t}{2\pi S}\int dq \sum_n \frac{1}{\sigma_{nq}}\left[\frac{|\Phi^2_{nq}|''}{2} + |\Phi^2_{nq}|\frac{(\epsilon'_{nq})^2 - (\sigma'_{nq})^2}{8\sigma^2_{nq}} - \frac{|\Phi^2_{nq}|'\sigma'_{nq}}{2\sigma_{nq}}\right] \quad , \tag{16}$$

$$L = \frac{n_b t\pi}{S^2 d} \quad , \tag{17}$$

where $t = 1/2\pi N_2 V^2$, $S = \frac{1}{2\pi}\int dq \sum_n |\Phi_{nq}|^2$. Notice that $\mathcal{D}$ and L are equivalent to the quantities $D\tau$ and τ, respectively, in weak localization: D being the diffusion coefficient and τ^{-1} the total impurity scattering rate.

If we assume that there is no reflection symmetry along the z direction, as e.g. in the (111) direction of GaAs[5] then $\epsilon_{n,-q} \neq \epsilon_{nq}$ and $\Phi_{n,-q} \neq \Phi_{nq}$ in general. As a consequence, a term linear in Q appears in the denominator of the Cooperon, multiplied by a coefficient B, where

$$B = \frac{i}{2\pi S}\int dq \sum_n \frac{|\Phi_{nq}|^2 \epsilon'_{nq}}{\sigma_{nq}} \quad . \tag{18}$$

However we will not refer further to this case.

Using these expressions, we obtain for the corrections to the conductivity

$$\delta\sigma_{xx} = -\frac{e^2V^2}{2\pi^2}\sum_{n,m}\int dq \; \frac{|\Phi_{nq}|^2|\Phi_{mq}|^2}{(\varepsilon_{nq}-\varepsilon_{mq})^2+(\sigma_{nq}+\sigma_{mq})^2} \; \left\{\frac{\epsilon_F-\varepsilon_{nq}}{\sigma_{nq}} + \frac{\epsilon_F-\varepsilon_{mq}}{\sigma_{mq}} + 3\,M_{nmq}\right\} \; I \tag{19}$$

$$\begin{aligned} M_{nmq} &= \frac{(\varepsilon_{mq}-\varepsilon_{nq})\;(\sigma_{mq}-\sigma_{nq})}{(\varepsilon_{nq}-\varepsilon_{mq})^2+(\sigma_{nq}-\sigma_{mq})^2} \; , \; m \neq n \; , \\ &= \frac{\epsilon'_{nq}\;\sigma'_{nq}}{(\epsilon'_{nq})^2+(\sigma'_{nq})^2} \; , \; m = n \;\; , \end{aligned}$$

$$\delta\sigma_{zz} = -\frac{m\,e^2V^2}{2\pi^2}\sum_{n,l}\int dq\;|\Phi_{nq}|^2|\Phi_{lq}|^2 \frac{\epsilon'_{nq}\;\epsilon'_{lq}\;(\frac{1}{\sigma_{nq}}+\frac{1}{\sigma_{lq}})}{(\varepsilon_{nq}-\varepsilon_{lq})^2+(\sigma_{nq}+\sigma_{lq})^2} \;\; I \;\; , \tag{20}$$

with

$$I = \frac{2L^{1/2}\tau_\phi^{-1/2}(T)}{\pi\sqrt{\mathcal{D}^2\;\mathcal{D}_z}} \arctan\sqrt{\frac{L\tau_\phi^{-1}(T)}{\mathcal{D}_z q_m^2}} \quad . \tag{21}$$

$q_m = \pi/d$ and $\tau_\phi^{-1}(T)$ is the dephasing rate of the Cooperon[1], arising from electron-phonon, electron-electron interactions etc. $\tau_\phi^{-1}(T)$ enters in the Cooperon in the following manner: $C(K,Q,\omega)^{-1} \to C(K,Q,\omega)^{-1} + \tau_\phi^{-1}(T)L$, where C is given by eq. (14). I has the limiting forms

$$I = \frac{L^{1/2}}{\sqrt{\mathcal{D}^2\;\mathcal{D}_z\;\tau_\phi(T)}} \quad , \quad L\tau_\phi^{-1}(T) \gg \mathcal{D}_z q_m^2 \quad , \tag{22}$$

$$I = \frac{2}{\pi\mathcal{D}\;\mathcal{D}_z q_m \tau_\phi(T)} \quad , \quad L\tau_\phi^{-1}(T) \ll \mathcal{D}_z q_m^2 \quad . \tag{23}$$

Weak disorder of bulk type, i.e. spreading over the whole volume, in superlattices was investigated e.g. in ref.[6], and our result for I is the same, in the limit $L\tau_\phi^{-1}(T) \gg \mathcal{D}_z q_m^2$. However, here the prefactors to the conductivity corrections as well as the coefficients $\mathcal{D}, \mathcal{D}_z$ and L are different, due to the fact that we are considering 'planar' disorder.

Let us note here that the above results for interface scattering were used in our work[7] on positive giant magnetoresistance, emanating from interactions and weak disorder.

a function of the field

$$I = \frac{\sqrt{eH}}{4\pi^2\sqrt{\mathcal{D}\mathcal{D}_z}}\sum_{n=0}^{N_H} b_n\;\arctan(b_n q_o) \quad , \quad b_n = \left(\frac{1}{aH}+n+\frac{1}{2}\right)^{-1/2} \quad . \tag{24}$$

Here $a = 4\mathcal{D}e\tau_\phi(T)/L$, $N_H = [q_o^2/\pi^2]$ and $q_o = \pi/(2\sqrt{eH\mathcal{D}})$. In contrast to this, the Drude term has a $(\omega_c\tau)^2 \ll 1$ field dependence, with ω_c being the cyclotron energy. Our results are relevant e.g. to the study of Cu/Al multilayers[8].

In the case of two planes per period situated in positions c and c', the potential (4) acquires another identical term with the argument c' in Φ. Henceforth we set

$$\Phi_{1nq} = \Phi_{nq}(c) \quad , \quad \Phi_{2nq} = \Phi_{nq}(c') \quad . \tag{25}$$

As a result, the denominator of the Cooperon contains now the constant term $1-A$ with

$$A=\sum_n\int dq\;\frac{|\Phi_{1nq}|^4+|\Phi_{2nq}|^4+2|\Phi_{1nq}|^2|\Phi_{1nq}|^2}{\sum_l\left\{|\Phi_{1nq}|^2|\Phi_{1lq}|^2+|\Phi_{2nq}|^2|\Phi_{2lq}|^2+2\Re\left[\Phi^*_{1nq}\Phi_{2nq}\Phi_{1lq}\Phi^*_{2lq}\right]\right\}}\quad . \tag{26}$$

In this way the Cooperon now is written as

$$C(K,Q,\omega)=\frac{1}{1-A+\mathcal{D}K^2+\mathcal{D}_zQ^2-i\omega L+\tau_\phi^{-1}(T)L}\quad , \tag{27}$$

with

$$\mathcal{D}=\frac{t^2}{4m\pi\, S^3}\int dq\sum_n\frac{\{\epsilon_F-\epsilon_{nq}\}[|\Phi_{1nq}|^4+|\Phi_{2nq}|^4]}{[|\Phi_{1nq}|^2+|\Phi_{2nq}|^2]^3}\quad , \tag{28}$$

$$\begin{aligned}\mathcal{D}_z=\frac{t}{2\pi S}\int dq\sum_n\frac{1}{\sigma_{nq}}\Bigg[&\frac{|\Phi^2_{1nq}|''+|\Phi^2_{2nq}|''}{2}+\{|\Phi^2_{1nq}|+|\Phi^2_{2nq}|\}\frac{(\epsilon'_{nq})^2-(\sigma'_{nq})^2}{8\sigma^2_{nq}}\\&-\frac{\{|\Phi^2_{1nq}|'+|\Phi^2_{2nq}|'\}\;\sigma'_{nq}}{2\sigma_{nq}}\Bigg]\quad ,\end{aligned} \tag{29}$$

$$L=\frac{t}{S^2}\int dq\sum_n\frac{|\Phi_{1nq}|^4+|\Phi_{2nq}|^4}{[|\Phi_{1nq}|^2+|\Phi_{2nq}|^2]^2}\quad . \tag{30}$$

Generally, this will result in the incomplete cancellation of the unity in the denominator of the Cooperon. This remaining term is equivalent to an effective temperature independent "dephasing rate" or mass term

$$\tau^{-1}_{\phi,eff}=\frac{1-A}{L}\quad . \tag{31}$$

If $\tau^{-1}_{\phi,eff}\gg\tau_\phi^{-1}$ the usual weak localization signature disappears. In that case, the diffusive behavior induced by one plane in the unit cell is washed out by the presence of the second plane, which in a way 'undoes' the effect of the former.

In summary, we provide an analysis of weak disorder effects from planar disorder in superlattices, which is equivalent to bulk-type disorder. We present and contrast the results from a single scattering plane per period vs. two scattering planes per period.

* E-mail : kast@iesl.forth.gr

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